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Activation of CH Bonds of Cyclohexane and Aromatic Hydrocarbons with Bis(picoline)dichloropalladium(II) in Nonpolar Solvents

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Abstract

Dichlorobis(picoline)palladium(II) complexes PdCl2(pic)2 (pic = β- or γ-picoline) were prepared and studied in reactions with cyclohexane, benzene, toluene, and o-xylene. At 120°C these hydrocarbons are converted to corresponding monochloro derivatives (chlorocyclohexane, chlorobenzene, and isomers of chlorotoluene and chloroxylene), and the palladium complex is reduced to form metallic palladium, picoline, and picolinium chloride. The initial rates of these reactions were estimated. The most active are toluene and xylene, benzene has the lowest activity, and cyclohexane has the intermediate activity. The addition of iodine to the reaction mixture revealed no organopalladium compounds. The reaction mechanism was studied. The activation of the hydrocarbons by oxidative addition to the palladium complex via CH bonds was proposed.